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**MONTE CARLO PWR CAVITY DOSIMETRY CALCULATIONS USING AN
AUTOMATIC VARIANCE REDUCTION TECHNIQUE**

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ABSTRACT

Although the Monte Carlo method is considered to be the most accurate method available for solving radiation transport problems, its applicability is limited by its exorbitant computational expensive. Thus, variance reduction techniques, which require intuition, guess work, and iterations involving manual adjustments, are employed to make reactor calculations feasible. Responding to this difficulty, we have developed methodology for automatic variance reduction of Monte Carlo shielding calculations using the discrete ordinates adjoint function for source biasing and consistent transport biasing with the weight window technique. We briefly describe the implementation of this method into the standard production Monte Carlo code MCNP, and its application to the cavity dosimetry calculation. The use of this method is shown to increase the calculational efficiency of the cavity dosimetry calculation by more than a factor of 4 and improve the statistical convergence, with respect to our best manually optimized model.

I. INTRODUCTION

The life of a reactor and its possible extension are directly dependent on the embrittlement of the reactor pressure vessel (RPV) under neutron irradiation. The embrittlement of the RPV material is due, primarily, to the bombardment of neutrons with energies greater than ~ 1 MeV, and cannot be directly determined from measured quantities. Radiation detectors are employed to provide data by which calculational methods/models can be verified. The dosimeters can be located both inside (in-vessel capsule) and outside (cavity dosimetry) the RPV. However, due to mechanical problems and subsequent safety issues, in-vessel capsules are no longer used in some of the US reactors. The cavity dosimetry calculations attempt to estimate high-energy (≥ 1.0 MeV) reaction rates in a small volume at a distance of ~ 350 cm from the core centerline, and are used to estimate RPV integrity and provide a basis for plant life extension. In the past, the discrete ordinates (S_N) method was used, almost exclusively, to perform these calculations. More recently, the Monte Carlo (MC) method has been employed for this application in an effort to better understand the uncertainties associated with the S_N method and to attempt to benchmark S_N calculations.[1, 2]

For many applications, such as the cavity dosimetry calculation, the computer time required by the analog MC method is prohibitive. Consequently, some form of variance reduction (VR) or biasing must be applied. The application of VR techniques can be quite difficult for cavity dosimetry problems that are complex and three-dimensional. An iterative process is typically employed to develop the VR parameters; converging at some acceptable level of calculational efficiency. Unfortunately, the appropriate VR parameters can vary significantly with the objective (e.g., dosimeter response function, location, etc.). Therefore, the iterative steps must be repeated for calculations with different objectives. Automatic importance generators, such as the weight window generator in MCNP[3], are currently available, but are restricted by their statistical nature and are of limited use in multi-dimensional deep-penetration problems. In the absence of more sophisticated methods, however, the weight window generator is a very useful tool in determining the VR parameters.[4]

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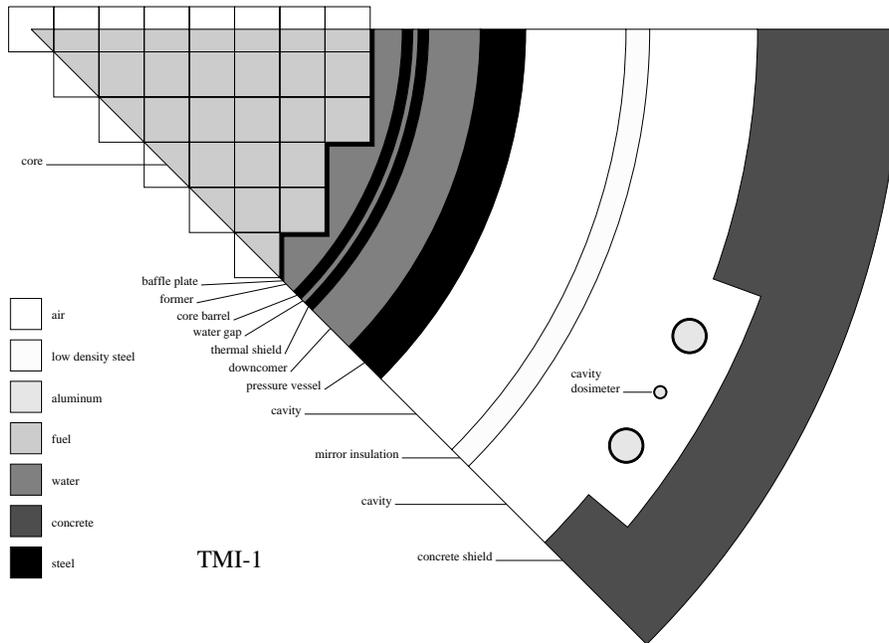


Figure 1: One Octant of the Three Mile Island unit 1 (TMI-1) Reactor

A further difficulty lies in the statistical convergence of the MC results. For large complex applications, it is not uncommon to spend days (and possibly weeks) iterating and adjusting the VR parameters only to achieve reasonable efficiency with unstable statistical behavior. This unstable statistical behavior is caused by improper use of the VR techniques (i.e., insufficient detail and/or inappropriate selection of the parameters) and is usually the result of undersampling some important region of the problem phase-space.[5] Further, this undersampling is often difficult to identify and correct.

It has long been recognized that the adjoint function (i.e., the solution to the adjoint Boltzmann transport equation) has physical significance as a measure of the importance of a particle to some objective function (e.g., the response of a detector)[6]. It is this physical interpretation that, in theory, makes the adjoint function well suited for use as an importance function for biasing certain types of MC calculations. Specifically, problems involving a small detector region(s) at a large distance from the source, such as the reactor cavity dosimetry calculation which attempts to estimate reaction rates at a distance of approximately 350cm from the core centerline. The problem is illustrated in Fig. 1, which shows one octant of the Three Mile Island unit 1 (TMI-1) reactor. MC and S_N models for this calculation are described in Refs. [1, 2] and [7], respectively.

In this paper, we demonstrate a method for using the S_N adjoint function for automatic VR of MC calculations through source biasing and consistent transport process biasing using the weight window technique. This method is applied to the cavity dosimetry calculation, and the increase in calculational efficiency is quantified.

II. THEORY

From adjoint transport theory[6], the response R at a detector is given by $R = \langle \phi^\dagger q \rangle$, where q is the source density, ϕ^\dagger is the adjoint function, and $\langle \rangle$ signify integration over all the independent variables. For the acceleration of this calculation, we use ϕ^\dagger to bias the source of particles as well as the transport of the particles through the medium. The source energy and position are sampled from a biased probability distribution function (*pdf*) $\hat{q}(r, E)$ given by,

$$\hat{q}(r, E) = \frac{\phi^\dagger(r, E)q(r, E)}{R}. \quad (1)$$

Physically, the numerator is the detector response from the space-energy element (dV, dE) , and the denominator is the total detector response R . Therefore, the ratio is a measure of the contribution to the detector response.

Since the source variables are sampled from a biased pdf , the statistical weight of the source particles must be corrected. This leads to the following expression for the statistical weight of the particles[8]

$$W(r, E) = \frac{R}{\phi^\dagger(r, E)} = \frac{q(r, E)}{\hat{q}(r, E)}. \quad (2)$$

To use the weight window facilities within MCNP, we calculate weight window lower bounds W_l such that the statistical weights defined in (Eq. 2) are at the center of the weight windows (intervals). The width of the interval is controlled by the parameter C_u , which is the ratio of upper and lower weight window values ($C_u = \frac{W_u}{W_l}$). Therefore, the weight window lower bounds W_l are given by

$$W_l(r, E) = \frac{W}{\left(\frac{C_u+1}{2}\right)}. \quad (3)$$

It is important to note that the expressions for the source biasing parameters and weight window lower bounds are consistent, and thus the statistical weights of the source particles are within the weight windows as desired. If the statistical weights of the source particles are not within the weight windows, the particles will immediately be split or rouletted in an effort to bring their weights into the weight windows.[3] This will result in unnecessary splitting/rouletting and a corresponding degradation in computational efficiency. For problems such as the cavity dosimetry calculation, where the adjoint function can vary by several orders of magnitude within the source region, this coupling between source and transport biasing is critical.

III. IMPLEMENTATION INTO MCNP

A. Overlay of Importance Function

The general version of MCNP provides facilities for energy and cell dependent weight windows. In order to use a fine spatial weight window grid (which is necessary in optically thick regions), the user must subdivide the cell based geometry such that the ratio of importances between adjacent geometric cells is not large. Because the importance ratios are not apriori known, this geometric discretization is not straightforward and typically requires iterations of adjustments. Further, the subdivision of the geometry into a very large number of cells is time consuming and can actually degrade the efficiency of the calculation. For these reasons, we use the S_N spatial mesh description to construct a separate, but related, geometric grid to facilitate the use of the adjoint distribution. This is done with a modified version of the MCNP code that is able to read the binary flux file (which contains the adjoint function and the spatial mesh and energy group information) from the standard S_N DORT code[9] and superimpose the variable spatial mesh and energy grid onto the MCNP problem.

B. Weight Checking

Various concepts for minimizing the amount of computational *overhead* associated with this process have been examined. An issue of concern is the determination of the appropriate time (or event) to check the particle's statistical weight. This is important for the following reasons: (1) because the MCNP geometry does not need to be manually subdivided to facilitate the spatial importances, the presently available weight checks (i.e., at collisions and surface crossings) are no longer sufficient to control particle weight and thus large differences in the weight scored by individual particles are possible, (2) there is a computational cost or penalty each time the weight is checked, and this penalty is the time required by the searching routines to determine the importance of the phase-space within which the particle resides, and (3) more frequent checking leads to more reliable results with well-behaved statistical convergence, but at some point the calculational efficiency is sacrificed. Therefore, it is clear that we need to determine an optimum or near-optimum criteria for checking particle statistical weights. Moreover, it is desirable that this criteria be problem independent.

Since the mean free path (mfp) is, by definition, the average distance a particle travels between collisions, it is a logical, problem independent parameter by which particle statistical weight can be controlled. Parametric studies analyzing the effect of the increment of mfp on problem efficiency and reliability[10] verify that a mfp increment of unity is a near-optimal problem-independent criteria for checking particle statistical weights.

IV. APPLICATION AND ANALYSIS

A. Application of Existing Variance Reduction Methods

Before the automatic VR method was developed and implemented into MCNP, the cavity dosimetry calculation was manually optimized with existing VR methods.[2] This manual optimization is now briefly described, and will be used as a reference for evaluating the automatic VR method.

MCNP (version 4A) offers several VR techniques that are applicable to the cavity dosimetry calculation. The techniques chosen for this application include: energy cutoff, source biasing, weight windows, and the exponential transformation. As the focus of the calculation is on high-energy neutrons that have experienced relatively few collisions, the energy cutoff was used to kill all particles with energies below 1 MeV and the MCNP default implicit capture was turned off. Source biasing was used to start more particles with high energies and desirable directions, and the source from the inner assemblies was neglected.[11] Weight windows were used to describe the spatial- and energy-dependent (2 energy groups) importance of the particles and to control particle weight fluctuations, and finally, the exponential transformation technique was employed in the steel regions to stretch the distance between collisions in the direction of interest.

Initially, geometric splitting was used to maintain a relatively constant flow of particles toward the cavity dosimeter. These geometric splitting parameters were then used in conjunction with the weight window generator to produce a spatial importance distribution for two energy groups. This process was extremely tedious, required many iterations of manually adjusting the weight window values, and a great deal of physical understanding. The manual process of optimization was continued until the desired level of efficiency was achieved (i.e., additional efforts were no longer productive) with stable statistical behavior.

B. Application of the Automatic VR Method

Because of the existence of measured data for the $^{63}\text{Cu}(n,\alpha)$, $^{58}\text{Ni}(n,p)$, and $^{54}\text{Fe}(n,p)$ reaction rates (responses), which have threshold energies of ~ 5.0 , ~ 1.0 , and ~ 1.0 MeV, respectively, all three reaction rates are of equal interest. Thus an effective response function (shown in Fig. 2) is calculated as the normalized sum of each of the normalized response functions. Using this effective response function, we can generate an importance function that will simultaneously optimize the calculation for all three reaction rates, and thus avoid calculating an importance function for each individual response that would require three separate MC calculations.

With this effective response function as the adjoint source, a 2-D R- θ adjoint function is calculated with the DORT code using the SAILOR P₃ 47-group library[12] and a symmetric S₈ quadrature set. Figure 3 shows this adjoint function distribution for energy group 3 (10.00-12.14 MeV). The modified version of MCNP reads the adjoint function, couples the original (MCNP) source distributions with the adjoint function to generate the source biasing parameters and weight window lower bounds, and then performs the transport calculation. The S_N spatial mesh which is used within MCNP to facilitate the spatial importance distribution is shown in Fig. 4. The following approximations/assumptions are made in this process: (1) the axial behavior for the adjoint function is approximated with a cosine distribution, and (2) to represent the spatial dependence of the energy biasing parameters, the energy dependent adjoint function is averaged over each user defined spatial source cell, and a dependent source energy biasing distribution is calculated for each source cell. For this particular application, each assembly has an associated source energy biasing distribution.

Since the focus of this paper is automatic VR for the MC cavity dosimetry calculation, the interested reader is referred to the references for discussions regarding the accuracy of results with respect to measurements and S_N calculations, as well as sensitivity studies related to various aspects of this calculation. However, to provide some indication of the accuracy, calculated-to-experimental (C/E) ratios, corresponding to ENDF/B-V material cross sections and SAILOR dosimetry cross-sections, are given in Table I. The differences between C/E ratios calculated with the manually optimized model and with the automatic VR method are within the statistical uncertainties.

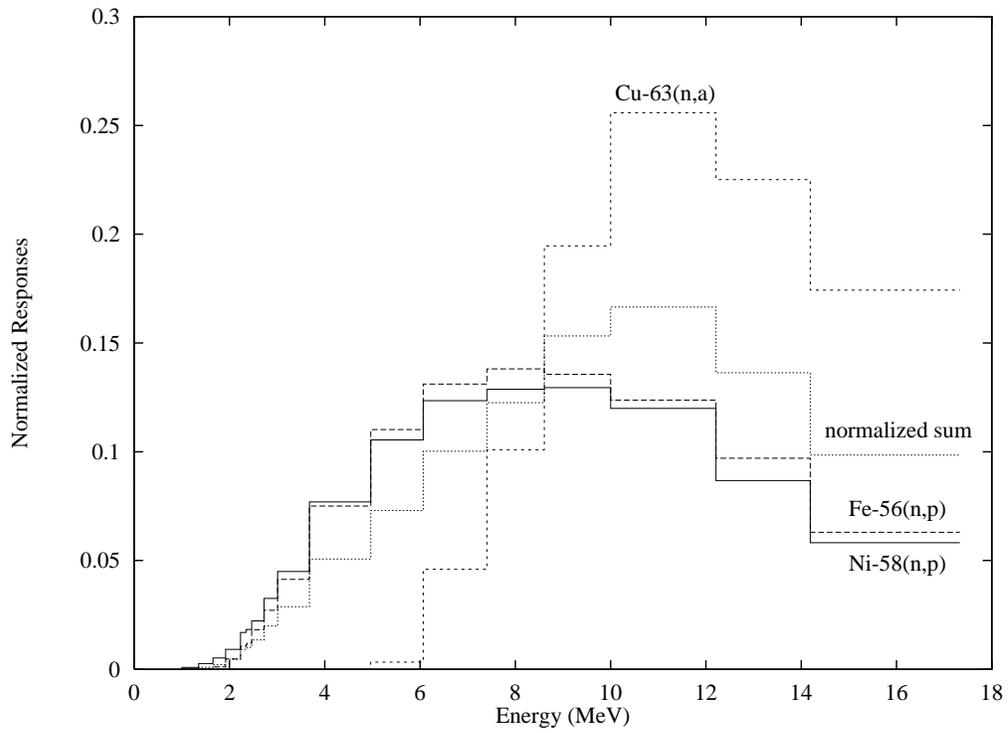


Figure 2: Response Functions

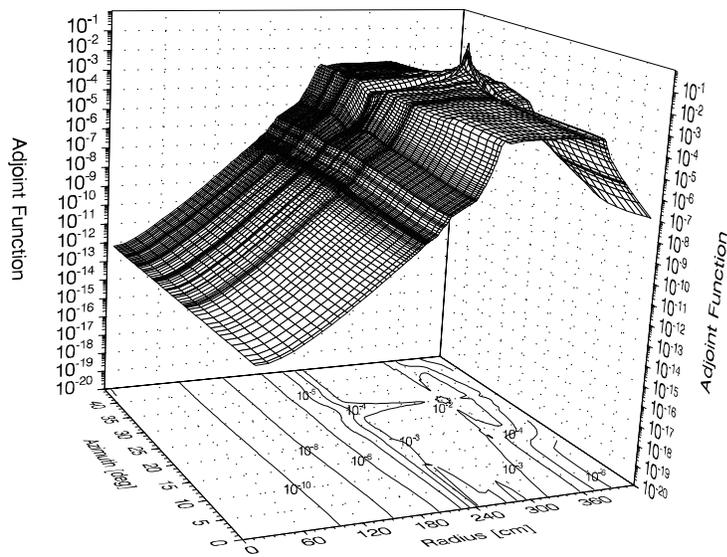


Figure 3: Adjoint Function Distribution for Energy Group 3 (10.00-12.14 MeV)

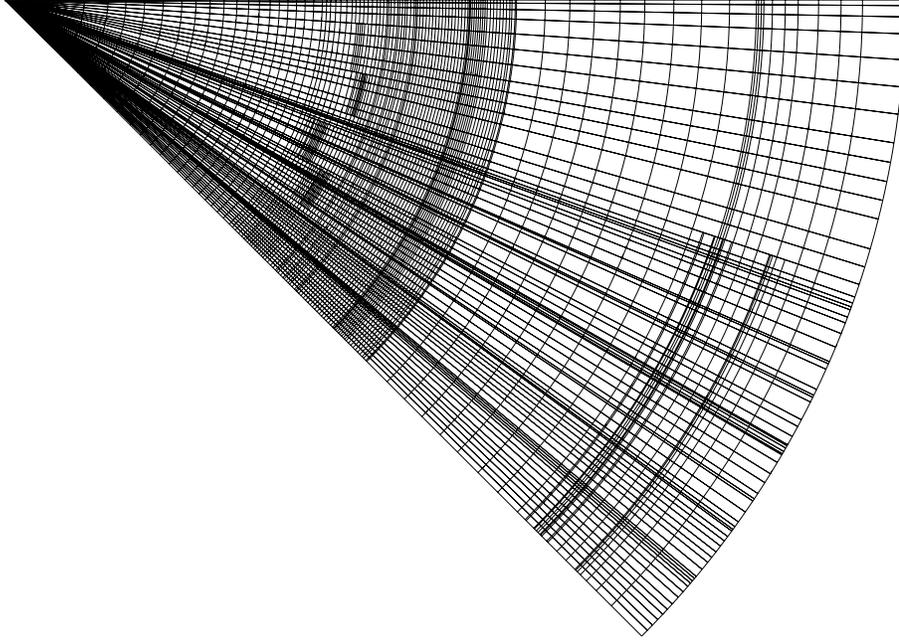


Figure 4: S_N Spatial Mesh Used to Facilitate the Spatial Importance Distribution

Table I: Calculated-to-Experimental (C/E) Ratios at the Cavity Dosimeter for TMI-1

Reaction	Manually Optimized		Automatic VR	
	C/E	FOM	C/E	FOM
$^{63}\text{Cu}(n,\alpha)$	0.905(0.022) ^a	3.7	0.878(0.022) ^a	16 (4.3) ^b
$^{54}\text{Fe}(n,p)$	0.965(0.023)	3.5	0.964(0.020)	20 (5.7)
$^{58}\text{Ni}(n,p)$	0.947(0.020)	4.5	0.952(0.019)	22 (4.9)

^a 1σ uncertainties

^b ratio of *Automatic VR* and *Manually Optimized* FOMs

C. Computational Efficiency

With the use of the automatic VR method, the computer time required by the MCNP model to calculate the reaction rates at the cavity dosimeter with 1σ uncertainties of less than 3% is ~ 1 hour on an IBM RISC/6000 model 370. To reach the same precision (3%) with the manually optimized model requires nearly 5 hours of CPU time. This behavior is demonstrated in Fig. 5 which plots relative error (RE) and $\frac{C}{\sqrt{T}}$ (where C is a constant and T is computer time) versus computer time for the three reaction rates of interest. The two sets of curves in Fig. 5 correspond to calculations performed with different VR approaches; namely, manually optimized VR and the automatic VR derived from a 2-D adjoint function distribution (18 energy groups) using the effective response function. To reach a 1σ relative error of $\sim 2\%$, the manually optimized and automatic VR cases require $20\text{E}+6$ and $3\text{E}+6$ particle histories, respectively.

One potential problem associated with the intense use of VR techniques is erratic or unreliable error estimations. Figure 5 shows that the RE follows the expected behavior predicted by the Central Limit Theorem ($RE \sim \frac{1}{\sqrt{N}} \sim \frac{1}{\sqrt{T}}$; where N is the number of particle histories), which provides some indication about the validity of the estimated RE. Moreover, the use of the automatic VR method appears to lead to smoother statistical convergence. All three reaction rate tallies pass all 10 of the MCNP statistical checks[3], providing an additional indication of proper

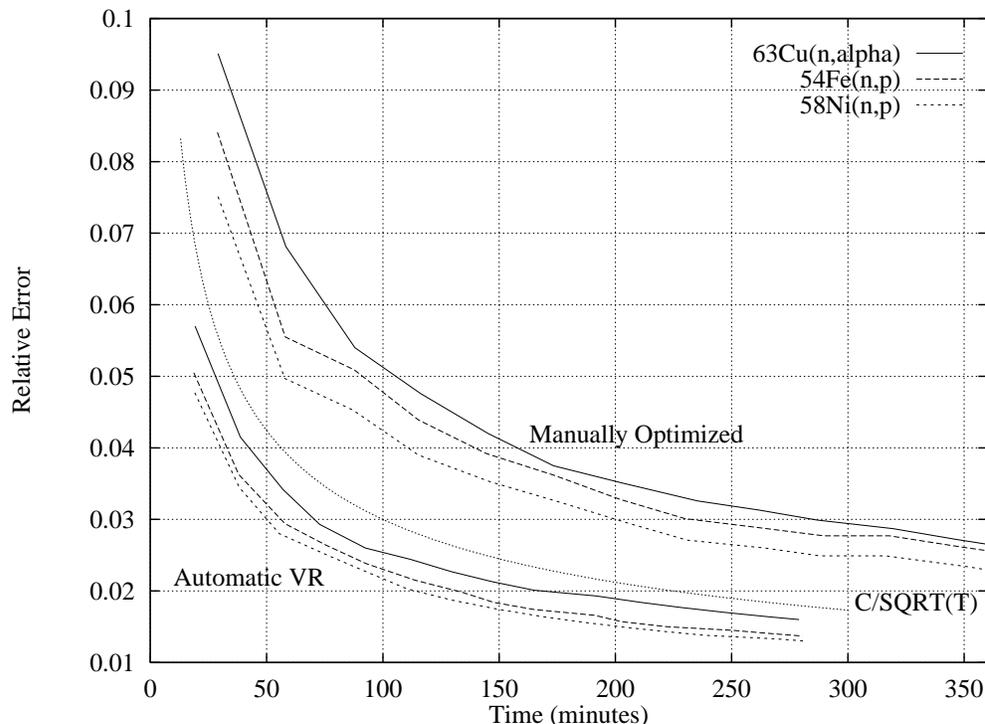


Figure 5: Relative Error vs Computer Time

Table II: Effect of Response Functions on FOMs at the Cavity Dosimeter for TMI-1

Reaction	effective response function		individual response functions	
	C/E	FOM	C/E	FOM
$^{63}\text{Cu}(n,\alpha)$	0.878(0.022) ^a	16 (4.3) ^b	0.890(0.033) ^a	25 (6.8) ^b
$^{54}\text{Fe}(n,p)$	0.964(0.020)	20 (5.7)	0.943(0.029)	25 (7.1)
$^{58}\text{Ni}(n,p)$	0.952(0.019)	22 (4.9)	0.933(0.026)	28 (6.2)

^a 1 σ uncertainties

^b ratio of *Automatic VR* and *Manually Optimized* FOMs

statistical convergence. Further analysis of the estimated uncertainties[8] has demonstrated that the estimated REs from the automatic VR case are much more reliable than those from the manually optimized case.

Table I lists Figure-Of-Merit (FOM) values [$FOM = 1/(R)^2T$] for the manually optimized calculation and the automatic VR calculation using a single effective response function. The use of the automatic VR method with an effective response function is shown to increase the calculational efficiency by more than a factor of 4 with respect to our *best* manually optimized importance function.

To evaluate the use of the effective response function, automatic VR MC calculations were also performed for each individual response function separately (i.e., an adjoint calculation was performed with each response function and used in individual MCNP calculations). Table II lists the FOM values for these calculations. The use of individual adjoint functions is shown to increase the efficiency by a factor of ~ 7 with respect to the single manually optimized importance function and by $\sim 35\%$ with respect to the adjoint function with an effective response function.

The aforementioned computer times do not include the S_N adjoint calculation. Also, for the purpose of comparison, the S_N reaction rate calculation (18 group, $E > 1.0\text{MeV}$) requires 3 individual DORT calculations, $R-\Theta$, $R-Z$, and R ; which require ~ 40 minutes of total computer time.

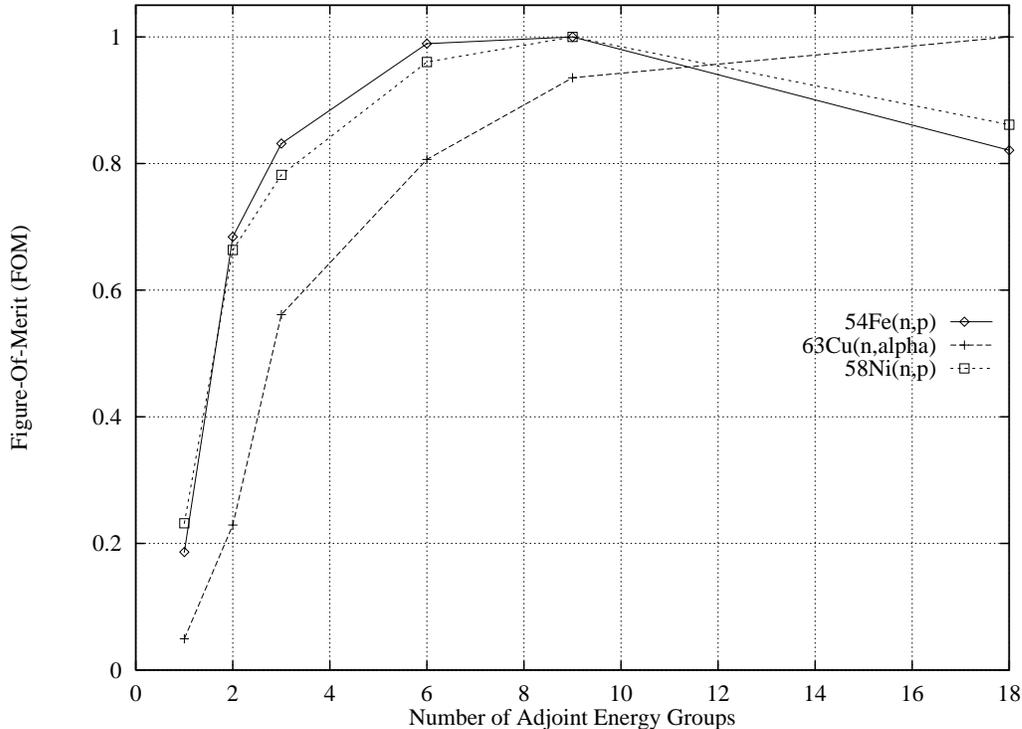


Figure 6: Effect of Number of Adjoint Energy Groups on FOM

D. Effect of Adjoint Accuracy on Calculational Efficiency

The effectiveness of an adjoint (importance) function for VR of MC calculations is dictated by its accuracy. It is for this reason that we use an accurate method - the S_N method - to calculate the adjoint function. However, for large problems such as this, and particularly for the extension to three-dimensional adjoint functions, the memory and disk space requirements for the S_N adjoint calculations can become prohibitive. One way to alleviate this problem is to sacrifice some of the accuracy of the adjoint calculation through the use of fewer energy groups. However, the relationship between the accuracy of adjoint functions and their effectiveness for VR of MC cavity dosimetry calculations is not well known.

To investigate the effectiveness of importance functions with varying degrees of energy-dependent accuracy, the 18-group (energy groups above 1 MeV) adjoint is collapsed[8] into 9-, 6-, 3-, 2-, and 1-group adjoint functions. The coarse group boundaries are a subset of the fine-group boundaries, and each coarse group contains the same number of fine groups. For example, in the 6-group structure, the highest energy group contains the highest three groups of the 18-group structure.

Figure 6 shows the relationship between the number of adjoint energy groups and the MC calculational efficiency, in terms of FOM. The FOM values are normalized such that the highest value is unity. The figure demonstrates that for this calculation there is no benefit to using more than ~ 9 groups. Further, while relatively minor losses in efficiency are associated with using fewer energy groups for the $^{54}\text{Fe}(n,p)$ and $^{58}\text{Ni}(n,p)$ reaction rates, large losses are observed for the $^{63}\text{Cu}(n,\alpha)$ reaction rate, which is sensitive to a rather narrow energy range ($\sim 6-12$ MeV). Nevertheless, for this particular problem an adjoint with relatively few energy groups (~ 3 groups) is capable of increasing the calculational efficiency to approximately half of the observed maximum, which is a factor of $\sim 10^4$ more efficient than the analog case.

V. SUMMARY

A general method for automatic VR of MC shielding calculations through source biasing and consistent transport process biasing has been presented. This method is implemented into the general purpose MC code MCNP and

applied to the reactor cavity dosimetry calculation. The use of this automatic VR method is shown to increase the efficiency of the reaction rate calculation by more than a factor of 4, with respect to our *best* manually optimized model, and produce more reliable error estimates. Further, this method does not require the intuition, guess work, and/or manual intervention typical of current VR techniques (or importance function generators), thus significantly reducing the analyst's time for performing these calculations.

The limitation to this approach is the requirement of an S_N adjoint solution. Therefore, strategies for generating input files for S_N calculations directly from MCNP input files are currently being developed. Coupling the work described in this paper with these strategies will result in the automation of the generation and application of the adjoint function for VR in MCNP calculations.

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